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VARIATIONAL METHOD IN THE STATISTICAL THEORY OF TURBULENT TWO-PHASE FLOWS

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Variational principles are introduced in the statistical theory of turbulent two-phase flows. With the help of these, correlation functions can be calculated by means of extremizing certain functionals. We carry out a sample calculation of the mean flow profile and correlation functions of a cylindrically symmetric two-phase jet. A Rayleigh-Ritz method is used for the determination of the correlation functions. There is a reasonable agreement between the theoretical calculation and experimental data even with a rather simple choice of the trial functions.

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1. INTRODUCTION

Almost all flows of interest to ballisticians involve the presence of a second phase and turbulence. In the absence of theoretical or experimental insight into their dynamics, the adopted approach has been either to ignore the turbulence or use ad-hoc single-phase descriptions with a number of "adjustable" parameters. Many of these do not have a sound theoretical underpinning or involve extrapolations and are more in the nature of post-facto instead of predictive.

To establish better modeling and computational capability in this field, a research effort was undertaken to shed light on the interaction of particulate presence on turbulence and vice versa. The statistical theory of turbulence gives a reasonably accurate description of the measured average flows and correlation functions and can be extended to nonreactive two-phase flows. However, if the two phases consist of a gas and of a dispersed solid phase, the extension is not a straightforward one. In fact, it requires a certain amount of "coarse-graining," (i.e., spatial averaging); this question was discussed rather carefully by Besnard and Harlow (1988). Alternatively, one can describe the dispersed particulate phase by means of a Boltzmann equation (Domokos, Kovesi-Domokos, and Zoltani 1988a, 1988b). This has the advantage that, in terms of a Chapman-Enskog expansion, one can generate not only the Eulerian equations, (the result of coarse-graining) but, in principle, corrections of arbitrary order to it. The difficulty is that very soon one runs into substantial computational difficulties. Even with the help of modern computers, a straightforward approach to solving the resulting coupled set of equations can be very time consuming.

In a previous work (Domokos, Kovesi-Domokos, and Zoltani 1991) we proposed a series of variational principles in the framework of the statistical theory of single-phase turbulent flows, based upon the work of Martin, Siggia, and Rose (1973) and De Dominicis and Peliti (1978) (see also Domokos, Kovesi-Domokos, and Zoltani 1988a, 1988b). A variational principle has the advantage that there exist methods to extremize the functional in question which are very economical from the calculational point of view—the Rayleigh-Ritz method being the most notable one. (The disadvantage is, of course, that some insight is necessary in order to guess good trial functions; most of the time one proceeds by trial and error in several steps.) In Domokos, Kovesi-Domokos, and Zoltani (1991) we performed a sample

alculation in order to describe a single-phase, cylindrically symmetric jet. Despite the implicity of the trial functions and the small number of parameters, quite a reasonable greement with the data was achieved.

The purpose of the present work is to extend the calculation to nonreactive, two-phase lows. The plan of this report is the following: In the next section we briefly review the ormalism described in Domokos, Kovesi-Domokos, and Zoltani (1988a, 1988b, 1991). For he sake of brevity, we use a somewhat abstract notation—this makes the concepts and the structure of the formalism more transparent. In Section 3 we state the framework for the computation of two-phase flows. Section 4 contains a sample of calculations of some of the properties of a cylindrically symmetric two-phase jet and a comparison of the results with experimental data. Finally, Section 5 contains the conclusions.

2. THE FORMALISM

We consider a vector space of dynamical variables; X denotes a generic element of the vector space. In general, X is a function of space and time. For instance, X may stand for the six components of the velocity field of a two-phase flow at a given space-time point (i.e., three components of the velocity of the carrier fluid and three components of the velocity of the particulate component). We assume that X obeys an autonomous equation of motion of the form

$$\partial_t X + F[X] = f\,, \tag{1}$$

where the functional $F[X]$ may contain spatial derivatives, integrals over spatial coordinates, etc., but no integral over time and no time dependence either. Further, f is a Gaussian random force, with correlation operator K.

The generating functional of the correlation functions is given in terms of an arbitrary source, j:

$$Z[j] = \int D\chi \exp\left[-<\partial_t X - F \,|\, K(\partial_t X - F)> + <j \,|\, X>\right]. \tag{2}$$

Here < .|.> stands for a suitable scalar product over the vector space, including integration over space-time variables and summation over discrete components. The functional measure, $\int D\chi$, contains an infinite determinant, *viz.* det $(\partial_t - \delta F/\delta X)$, as explained in Domokos, Kovesi-Domokos, and Zoltani (1988a). The cumulants are generated by $W = -\ln Z$.

The various averages are obtained by taking functional derivatives of W with respect to j. We use the notation

$$G(1) \equiv \langle X(x_1) \rangle = \frac{\delta W}{\delta j(x_1)}, \tag{3}$$

$$G(1,2) \equiv \langle X(x_1) X(x_2) \rangle = \frac{\delta^2 W}{\delta j(x_1) \delta j(x_2)}, \tag{4}$$

and so on. Here x_i stands for a *space-time point*.

In order to get a suitable variational principle, we also add a bilinear source in the exponential of Equation 2, of the form, $\langle \eta(1,2) \mid G(2,1) \rangle$ (Domokos, Kovesi-Domokos, and Zoltani 1991). Next, we perform a double Legendre transformation in the variables j and η, so that the resulting functional has $G(1)$ and $G(2)$ as its functional arguments. We denote this functional by S.

One has the relations

$$\frac{\delta S}{\delta G(1)} = -j(1), \ \frac{\delta S}{\delta G(1,2)} = -\eta(1,2). \tag{5}$$

The functional given by Equation 5 is stationary if the arbitrary sources are put equal to zero. The reader will readily recognize that functionals of the type in Equation 5 play a role analogous to the entropy in statistical mechanics. For this reason, relations of the type 5 with vanishing external sources were called ***the principle of stationary entropy*** in an analogous context by De Dominicis and Martin (1964).

3. EQUATIONS FOR A TWO-PHASE TURBULENT FLOW

In what follows, variables characterizing the *carrier fluid* will be given a subscript *f*, those characterizing the *dispersed particulate phase* a subscript *p*. We work in terms of dimensionless variables by dividing velocities with some characteristic speed, coordinates by a characteristic size of the system under consideration, etc. In this report we write down the equations of motion in the leading approximation of the Chapman-Enskog expansion (Domokos, Kovesi-Domokos, and Zoltani 1988a) so that both phases obey the equations of hydrodynamics. The volume fractions of the fluid and particulate phase are denoted by ε_f and ε_p, respectively. Of course,

$$\varepsilon_f + \varepsilon_p = 1 . \tag{6}$$

We now have the equations of continuity,

$$\partial_t \varepsilon_f + \frac{\partial}{\partial x^i}\left(\varepsilon_f u_f^i\right) = 0 , \tag{7}$$

$$\partial_t \varepsilon_p + \frac{\partial}{\partial x^i}\left(\varepsilon_p u_p^i\right) = 0 . \tag{8}$$

The equations of motion read

$$\partial_t\left(\varepsilon_f u_f^i\right) + \frac{\partial}{\partial x^j}\left(\varepsilon_f u_f^i u_f^j\right) + \frac{\varepsilon_f}{\rho_f}\frac{\partial p}{\partial x^i} = \varepsilon_f \varepsilon_p \frac{C}{\rho_f}\left(u_p^i - u_f^i\right) + f_f^i , \tag{9}$$

$$\partial_t\left(\varepsilon_p u_p^i\right) + \frac{\partial}{\partial x^j}\left(\varepsilon_p u_p^i u_p^j\right) + \frac{\varepsilon_p}{\rho_p}\frac{\partial p}{\partial x^i} = \varepsilon_f \varepsilon_p \frac{C}{\rho_p}\left(u_f^i - u_p^i\right) + f_p^i . \tag{10}$$

Here f_f and f_p stand for the perturbing Gaussian random forces acting on the fluid and particulate phases, respectively. In Equations 9 and 10, *p* stands for the external pressure. The quantity *C*, in general, is a function of $|\, u_f - u_p \,|$. However, with the exception of some

unusual cases such as highly viscous carriers, very heavy loading, etc., the velocity difference between both phases is not too big. In that case, C can be, to a good approximation, replaced by its value given by Stokes' law. This results in a considerable simplification of the computations.

The reader will notice that a viscous term has been omitted from Equation 9. Despite the fact C is proportional to the viscosity of the carrier fluid, the approximation is a permissible one unless one is interested in very small scales (large wave numbers). The coupling term is proportional to a velocity difference (in the Stokesian approximation), whereas the viscous term is proportional to the scalar curvature of a velocity field (on large and moderate length scales, the latter is less important than the former).

Let us now take a look at Equations 6, 7, and 8. One immediately realizes that if the flow of one of the phases is approximated by an incompressible one, the flow of the other phase becomes incompressible too. In a large number of practically important situations, the approximation of an incompressible flow is a rather good one. In what follows, we are going to make the approximation. Approximating a flow by an incompressible one has two immediate consequences. First, the pressure is no longer an independent dynamical variable; it can be integrated out explicitly from the generating functional of the correlation functions.* Second, the equations of continuity now tell us $\nabla \cdot u_f = \nabla \cdot u_p = 0$; hence, the velocity fields can be obtained as curls of vector potentials with an ensuing gauge of freedom (Domokos, Kovesi-Domokos, and Zoltani 1991).

Finally, the expression of the stirring force (or, more precisely, its correlation operator) has to be discussed. In Section 4, and in many other practically important cases, we are concerned with problems where the mean flow is cylindrically symmetrical, with the mean velocity having a large component along the axis of symmetry and a rather small radial component. In such cases one gets satisfactory results by taking a stirring force of the same symmetry and, in fact, neglecting the radial component of the stirring force altogether. We take for both phases an identical form of the matrix elements of the correlation operator, *viz.*,

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* Traditionally, this is formulated as using the equations of motion to eliminate the pressure; however, within the present context, performing a Gaussian functional integral over the pressure leads to the desired result in a more transparent manner (Domokos, Kovesi-Domokos, and Zoltani 1991).

$$K_{i,j}(x,x') \propto \exp(-\alpha\,|x^3 - x'^3|)\,\delta^2(x_T - x'_T)\,\delta(t - t')\,\delta_{i,3}\delta_{j,3}, \tag{11}$$

where the axis of symmetry has been chosen as the *3ᵈ* axis and x_T denotes a vector lying in a plane perpendicular to it. The stream-wise correlation of the stirring force is governed by the parameter α. As it turns out, its magnitude is not a critical one (Burgett 1989), but it seems that letting $\alpha \to 0$ is not a very good approximation.

Now we have assembled the elements of computing the generalized entropy, Equation 5. We have done it to two-loop accuracy (Domokos, Kovesi-Domokos, and Zoltani 1991) (i.e., by computing the first approximation to the solution of the Cornwall-Jackiw-Tomboulis functional differential equation).

Unfortunately, the result of the calculation is neither transparent nor revealing. (In fact, most of the calculation has to be performed by means of symbolic manipulation programs.) The reader will be spared the sight of the result. Instead, in the next section, we present the results of a calculation of the correlation functions of a steady two-phase jet sufficiently far from the plane of injection. (In this way, one can assume that the turbulence is fully developed: transients died away and the correlation functions are stationary.)

4. CORRELATION FUNCTIONS OF A CYLINDRICALLY SYMMETRIC TWO-PHASE JET

The calculation of a cylindrically symmetric jet is of considerable practical importance—many jets possess, to a very good approximation, axial symmetry. In addition, it is a relatively simple configuration; it is eminently suitable for testing a method of calculation. We proceeded in a way which proved to be successful in our previous work. The procedure follows:

- The velocity fields are obtained as the curl of vector potentials: $u_{f,p} = \nabla \times A_{p,f}$.

  We work in an axial gauge: the component of the vector potential along the axis of symmetry (chosen to be the *3ᵈ* axis) vanishes.

- A Reynolds decomposition is used for the vector potentials: $A = \langle A \rangle + A'$ correspondingly, the velocity fields are decomposed as $u = U + u'$. (For the sake of simplicity, we omitted the indices *f,p*; the decomposition is used for both phases.)

- We determine the form of the correction functions of the vector potentials:

$$Z^{i,j}_{\alpha,\beta} = \delta_{\alpha,\beta} Z^{i,j}_1 + \varepsilon_{\alpha,\beta} Z^{i,j}_2 \,. \tag{12}$$

  In this equation, δ and ε stand for the Kronecker and Levi-Civita tensors, respectively. Lower case Greek indices refer to vector components in the plane transverse to the symmetry axis, the superscripts i, j assume the values f and p.

- One assumes a trial form of the vector potentials and of the functions $Z^{i,j}_{1,2}$ containing a few unknown parameters.
- These expressions are substituted into the expression of the effective Equation 5.
- The entropy is then extremized with respect to the parameters. This determines their optimal values given the functional form of the vector potentials and correlation functions.
- Finally, the mean velocities and correlation functions are computed by taking the appropriate curls.

(Extremizing the entropy with respect to parameters in a given functional form is the Rayleigh-Ritz method of solving a variational problem.)

All velocities are measured in units of the fluid velocity, U_0, on the axis at the plane of injection. The unit of length is the diameter of the injection pipe. All vector potentials and correlation functions are assumed to be time independent. We chose essentially the same trial functions for both phases as in the case of a single-phase flow. (Of course, the optimal values of the parameters are different.) We used the 3^d component of the mean velocity on the axis as an input. The data were taken from Zoltani and Bicen (1990). The following forms give a good fit to the data,

$$U^f_3(z, r = 0) = \frac{1.35}{1 + 0.035 z^{3/2}} - 0.35 \exp(-0.1 z^2) \,, \tag{13}$$

$$U^p_3(z, r = 0) = 0.78 \left(\frac{1.13}{1 + 0.007 z^{3/2}} - 0.13 \exp(-0.03 z^2) \right) . \tag{14}$$

The functional form of the average of the vector potential was assumed to have a Gaussian radial dependence for both phases. In cylindrical coordinates we have

$$\langle A_\phi \rangle = \frac{1}{2} R(z)^2 \exp\left(- \frac{r^2}{R(z)^2} \right) , \tag{15}$$

with $R(z) = a + bz$. The optimized values of the parameters a and b are

$$a_f = 0.25,\ b_f = 0.076\,;\ a_p = 1.38,\ b_p = 0.013\ .$$

Likewise, we used the same functional form for the quantity Z_1 as in Domokos, Kovesi-Domokos, and Zoltani (1991) for both phases

$$Z_1 = A \exp\left[-f(z_1 - z_2)^2 - g(x_{T,1} - x_{T,2})^2 \right]$$
$$\exp(-\delta M)(1 + BM)\left[U_3(z_1,0)\, U_3(z_2,0) \right]^{1/2} . \tag{16}$$

Here,

$$M = \frac{1}{2}\left[\frac{x_1^2 + y_1^2}{R(z_1)^2} + \frac{x_2^2 + y_2^2}{R(z_2)^2} \right].$$

(Just as in Domokos, Kovesi-Domokos, and Zoltani [1991], we set $Z_2 = 0$.) The optimal values of the parameters are

$$A^{f,f} \approx 0.0019, A^{p,p} \approx 0.0013, B^{f,f} \approx 2.3, B^{p,p} \approx 3.5, \delta^{f,f} = 1.79, \delta^{p,p} \approx 2.63\ .$$

The values of the parameters f, g are practically identical in both phases, $f^{p,p} \approx f^{f,f} \approx 5.6$ and $g^{p,p} \approx g^{f,f} \approx 3.7$. These values have been computed for the particle loading extracted from Zoltani and Bicen (1990). The cross correlation functions, $Z_1^{p,f}$, have basically the same shape (the parameters B, δ, f, g are practically identical). However, the overall scale is much

smaller ($A^{p,f} \ll A^{f,f}$). This is intuitively obvious—with the loading fraction used in Zoltani and Bicen (1990), the coupling between both phases is a rather weak one. As a consequence, it is rather hard to obtain a reliable estimate of $A^{p,f}$. Several iterations fluctuate around a value of the cross correlation scale at least an order of magnitude smaller than (the comparable) fluid and particle correlation scales; however, a stable maximum of the generalized entropy, Equation 5 is hard to achieve.

Once we have these parameters values, one can take the curl of the mean vector potential and the double curl (with respect to both arguments) of $Z_{\alpha,\beta}$ in order to obtain the mean velocity and the correlation functions of the fluctuations, respectively. Experimental data on the fluctuation correlation are often taken at coincident arguments; this was the case in Zoltani and Bicen (1990) too. We display the results for those correlation functions where data were available in those articles. The other correlation functions can be easily reproduced from the preceding formulae.

In the figures, we return to a conventional notation which is acceptable for coincident arguments. The correspondence between the present notation (more suitable for theoretical calculations) and the conventional one is the following. Define

$$G_{a,b} = [\overrightarrow{\nabla} \times Z \times \overleftarrow{\nabla}]_{a,b}, \tag{17}$$

(i.e., the double curl of the fluctuation correlation function of the vector potential with respect to both arguments). (In the case of coincident arguments, the *curls are taken before the arguments are let to coincide.*) Note that $G_{a,b}$ defined by Equation 17 is just the correlation function of velocity fluctuations. For the sake of simplicity, we omitted the indices refer to the phase (*f,p*) in question.

We now have the correspondence between the conventional notation and the one used here in Domokos, Kovesi-Domokos, and Zoltani (1991)

$$\frac{\langle (u)_f^2 \rangle}{U_0^2} = G_{3,3}^{f,f} \; , \tag{18}$$

and a similar relation for the particle-particle correlation function. In an arbitrary Cartesian coordinate system (the 3^d axis coinciding with the axis of symmetry and the orientation of the 1^{st} and 2^{nd} axes being determined by the measuring apparatus) the components in the plane perpendicular to the axis of symmetry are denoted by v and w, respectively. There is a relation between $\langle v^2 \rangle$, $\langle w^2 \rangle$, etc., and our notation similar to the one exhibited in Equation 18. It is an obvious one and we do not exhibit it here. Note that cylindrical symmetry entails

$$G_{1,1}^{i,j} = G_{2,2}^{i,j} , G_{1,2}^{i,j} = 0 \; , \tag{19}$$

for any combination of the phases p,f. (There is no good notation available in the conventional system of notations for correlation functions such as $G_{a,b}^{p,f}$. However, among the figures presented in the present work, no such correlation function has been plotted.)

5. CONCLUSIONS

The extension of the calculations described in Domokos, Kovesi-Domokos, and Zoltani (1991) to a two-phase flow have basically the same merits as in the case of a single-phase flow. One notes again that the variational method is a very economical one from the computational point of view. With rather simple functional forms of the trial functions and in terms of a few parameters, a reasonable agreement with the experimental data can be obtained at the cost of a relatively small computational effort.

One can conceive a number of ways in which the agreement with the experimental data could be improved.

- One can contemplate calculating higher order approximations to the generalized entropy (De Dominicis and Peliti 1978).
- One can invent (with some physical insight) more sophisticated trial functions for the description of the mean flows and the fluctuation correlation functions.

- Clearly, more experimental data are necessary in order to determine the dependence of the various correlation functions on such physical quantities as the loading fraction, the viscosity of the carrier fluid, etc. In turn, this will enhance one's physical insight in "guessing" more sophisticated trial functions in the Rayleigh-Ritz method.

At this point it is hard to determine the increase in computational cost once one decides to go beyond the present, simplest approach. Nevertheless, experience with variational methods in various branches of physics suggests that many methods are likely to be rather economical in the statistical theory of turbulence too.

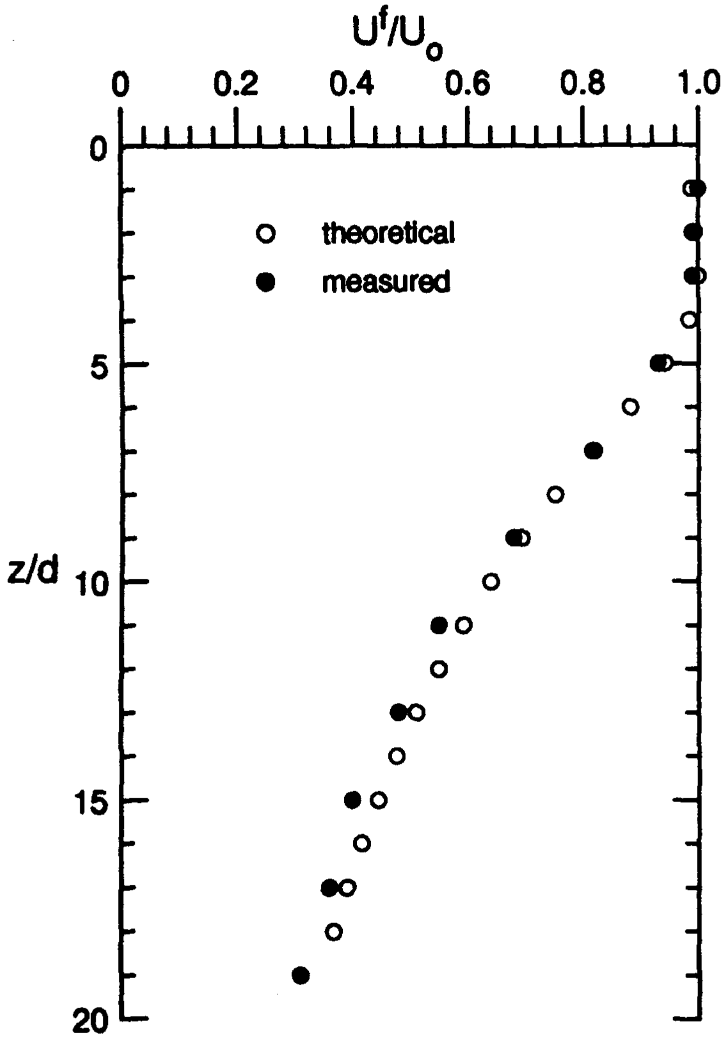

Figure 1. Mean Flow of Carrier Fluid at the Centerline of Jet, as a Function of the z Coordinate.

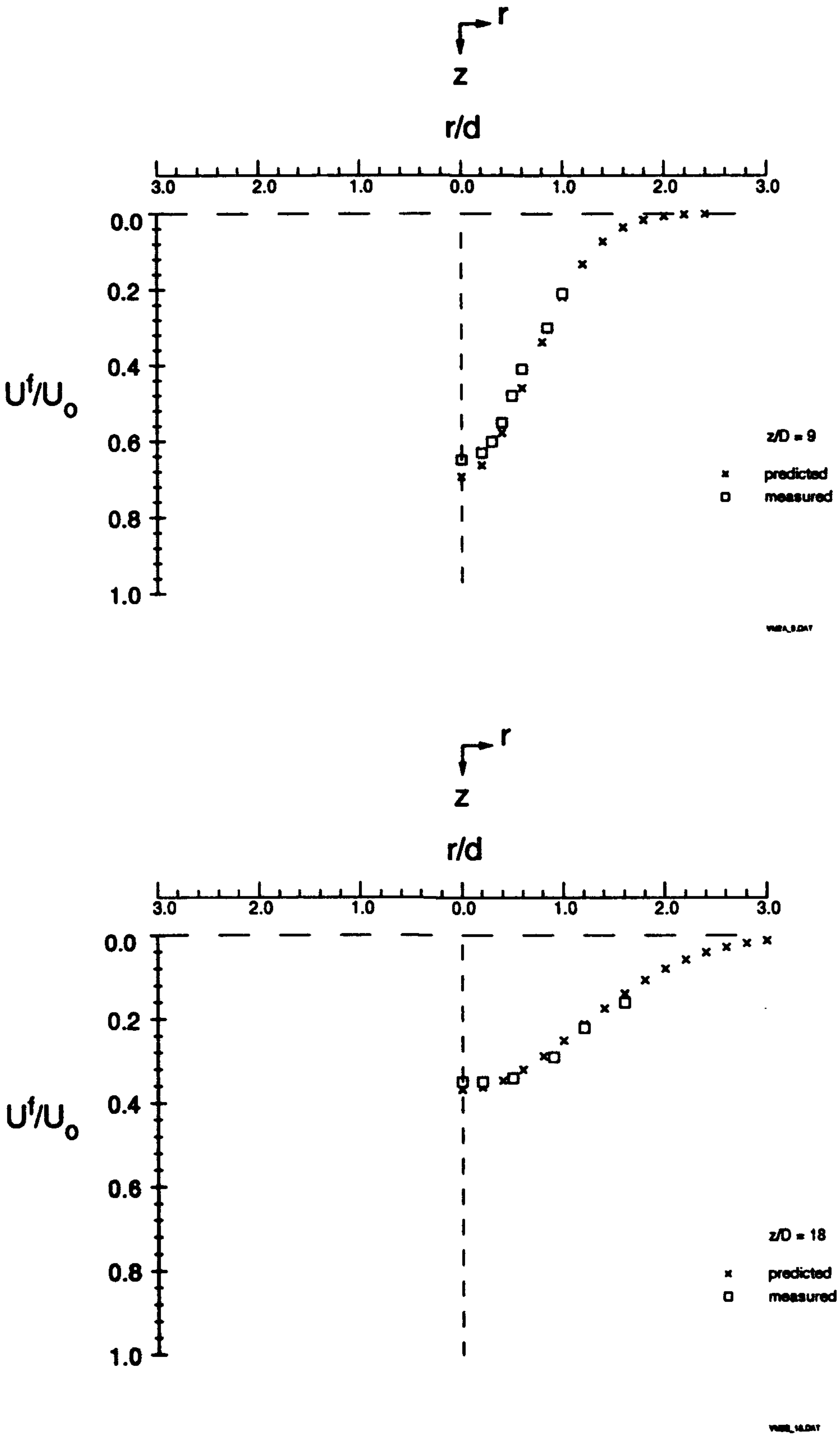

Figure 2. Mean Flow of the Carrier Fluid at Various Distances From the Jet Exit (Radial Component).

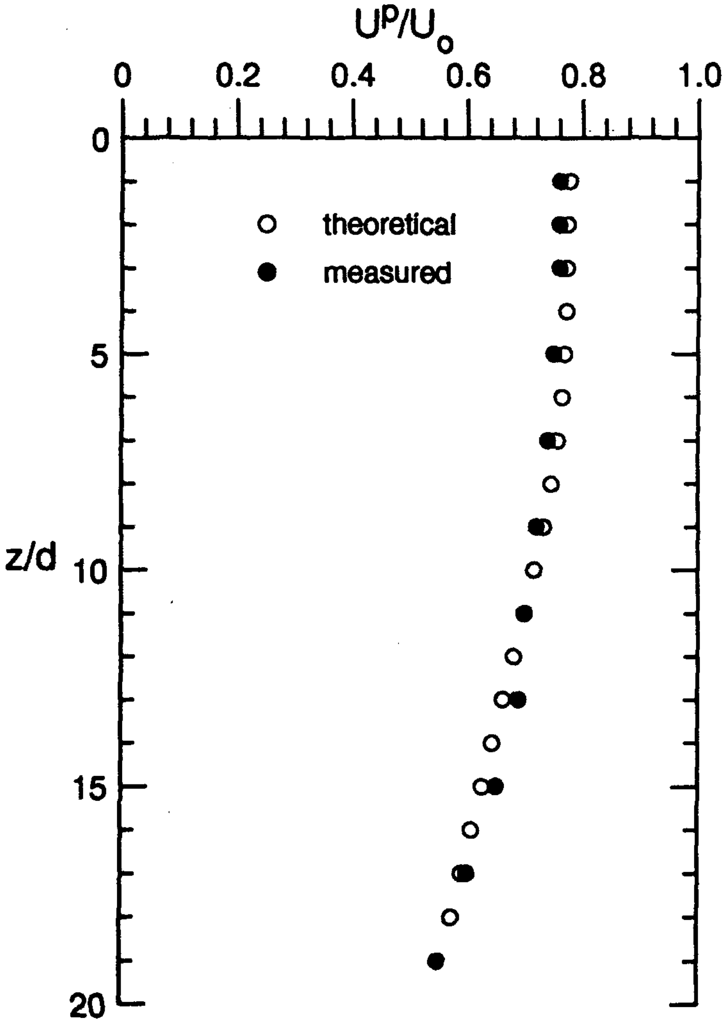

Figure 3. Mean Flow of the Particulate Phase at the Centerline of Jet, as a Function of the *z* Coordinate (Stream-Wise Component).

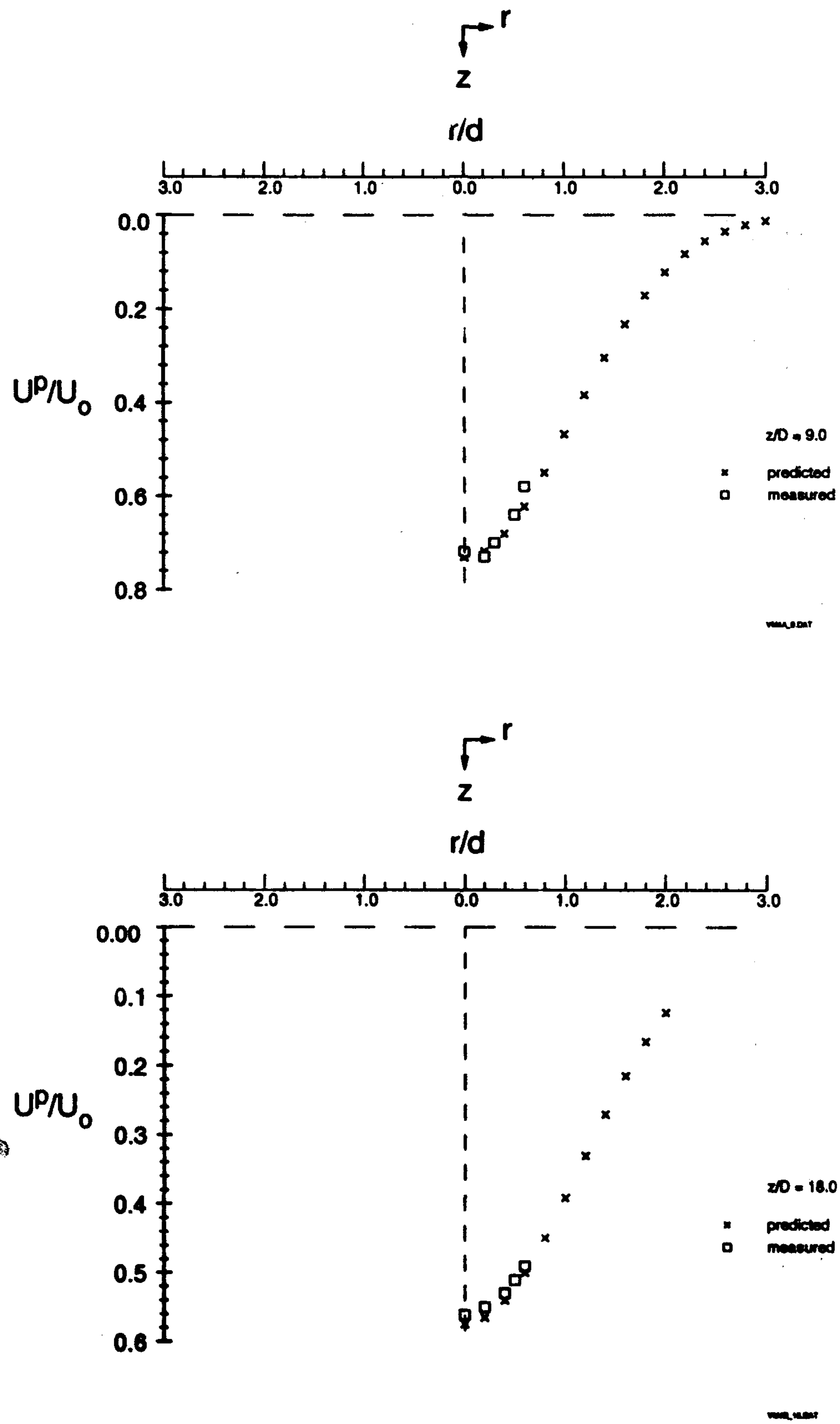

Figure 4. Mean Flow of the Particulate Phase at Various Distances From the Jet Exit (Radial Component).

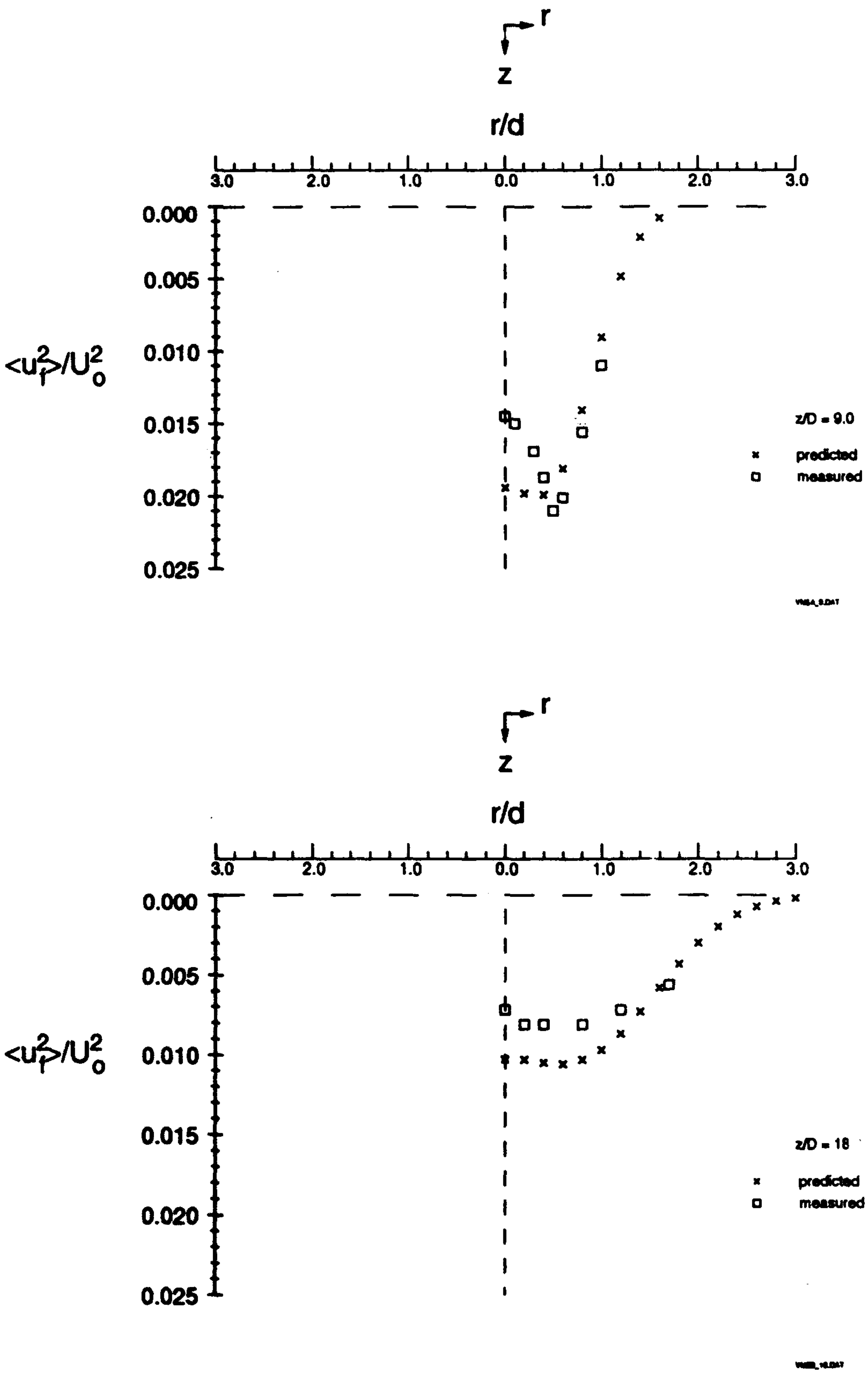

Figure 5. Fluctuation of the Stream-Wise Component of the Carrier Fluid at Various Distances From the Jet Exit.

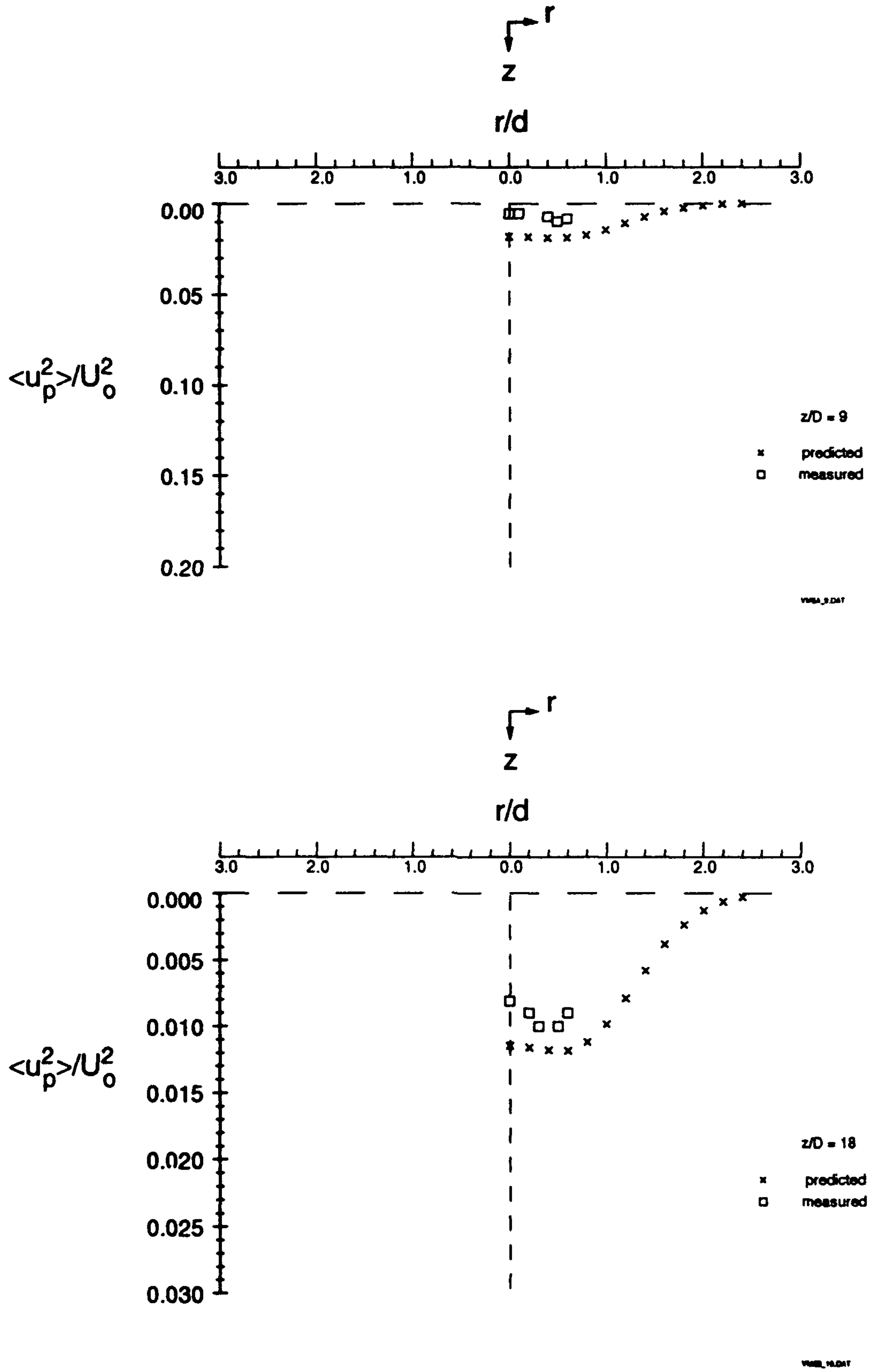

Figure 6. Fluctuation of the Stream-Wise Component of the Particulate Phase at Various Distances From the Jet Exit.

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